

**Comment on “First-principles studies on magnetic properties of rocksalt structure  
MC ( $M=\text{Ca, Sr, and Ba}$ ) under pressure”[Appl. Phys. Lett. 98,182501(2011)]**

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A recent Letter<sup>1</sup> reported magnetic properties and electronic structures of  $MC$  ( $M=\text{Ca}$ ,  $\text{Sr}$ , and  $\text{Ba}$ ) under pressure. As shown in Fig.1 in the Letter<sup>1</sup>, there are discontinuous jumps in the magnetic moment when the lattice constants are decreased. There is also intermediate spin magnetic moment in a quite wide range of the lattice constant in  $\text{SrC}$  and  $\text{CaC}$ . However, these results come from the inaccuracy of the calculation: the non-convergence of the spin moment with respect to the k-point mesh in the Brillouin zone.

With the input parameters provided by the authors, by using the same code we obtained that the spin moment are  $0.43$  and  $2.00 \mu_B$  when the lattice constants of  $\text{SrC}$  were set to  $4.70$  and  $5.67 \text{ \AA}$ , respectively, which are in agreement with the data in Fig.1 (a) of the Letter<sup>1</sup>. We can show that the mesh point number  $7 \times 7 \times 7$  in the work is much too few to converge the energy and spin moment under pressure. As shown in Fig.1, convergency of energy within  $1 \text{ meV}$  can only be achieved when the k-points are larger than  $20 \times 20 \times 20$  if the lattice constant is  $4.70 \text{ \AA}$ . The convergency is faster if the lattice constant is larger (e.g.  $5.67 \text{ \AA}$ ) where the half metallic character is present. This is mainly because of the metallic nature of the Fermi surface which requires much more k-points to converge<sup>2</sup>. The magnetic moment also changes significantly with the increasing k-points and converges to zero when the lattice constant is  $4.70 \text{ \AA}$  as shown in the figure with hollow circles.

We recalculated the magnetic moment at different lattice constants as shown in Fig.2 with the increased k-point number  $32 \times 32 \times 32$ . The spin magnetic moment decreases continually to zero when the lattice constant is decreased as shown in Fig.2. The decrease of the spin moment in  $\text{BaC}$  and  $\text{SrC}$  is faster than in  $\text{CaC}$ . There is an inflexion point when the lattice constant is  $8.2 \text{ a.u.}$  in the latter compound. The equation of state of the three compounds was obtained by differential of the energy with respect to the volume as shown in Fig.3( $\text{BaC}$ ) and Fig.4 ( $\text{CaC}$  and  $\text{SrC}$ ). There is hysteresis in the pressure-lattice constant curves for  $\text{BaC}$  which signatures a first order transition. This happens at  $p = 9.14 \text{ GPa}$  when the pressure is increased and at pressure  $p = 8.10 \text{ GPa}$  when the pressure is decreased. In the other two compounds, the lattice constant changes gradually with the pressure. However, a kink appears in  $\text{SrC}$  at pressure of  $56 \text{ GPa}$ .

## REFERENCES

<sup>1</sup>Shengjie Dong, Hui Zhao, Appl. Phys. Lett. **98**, 182501 (2011)

<sup>2</sup>R. M. Martin, Electronic Structure, Basic theory and practical methods, Cambridge Univ. Press., 2004

## FIGURES

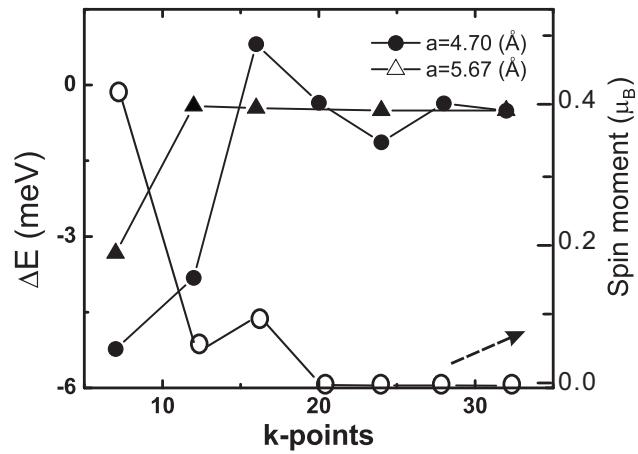


FIG. 1. The ground state energy at lattice constant of 4.70 Å (filled circles) and 5.67 Å (filled triangles) and the spin magnetic moment (hollow circles) at lattice constant of 4.70 Å after self-consistent calculations vs. k-points for SrC. The abscissa are the k-point in one direction of the Brillouin zone. The total number of the k-points is the cubic of the abscissa.

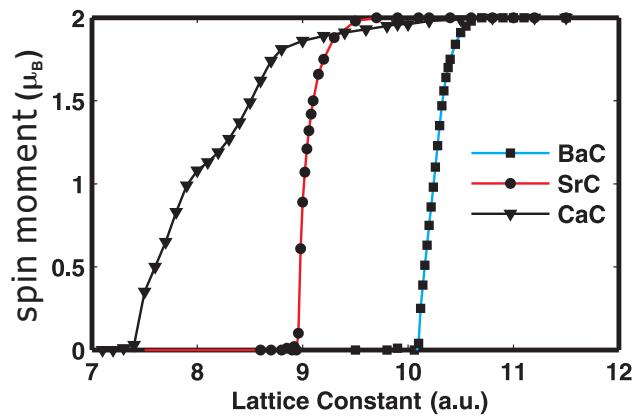


FIG. 2. The spin magnetic moment at different lattice constants of the three compounds.

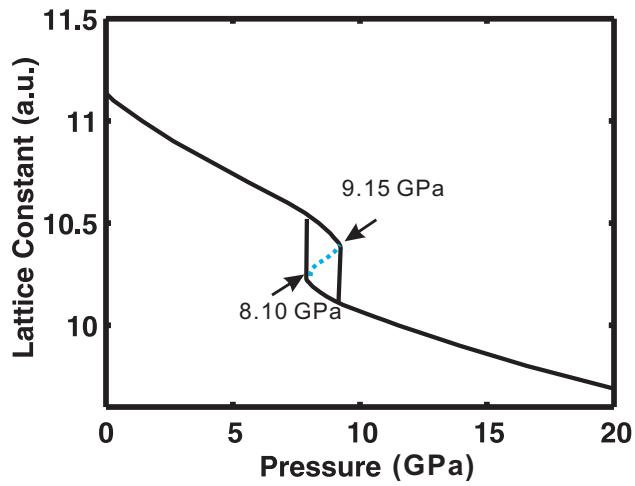


FIG. 3. The lattice constant vs. the hydrostatic pressure for BaC. The dashed line shows the path of the unstable state.

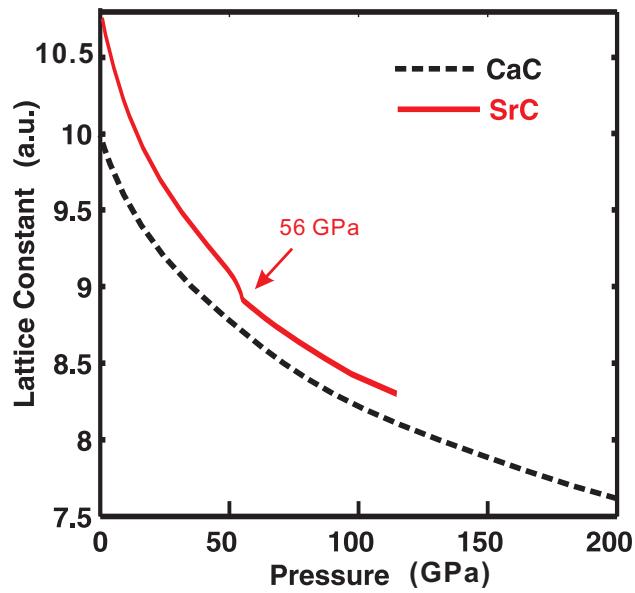


FIG. 4. The lattice constant vs. the hydrostatic pressure for SrC (solid lines) and CaC (dashed lines).